

## CORRECTION

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# Correction: Zn<sup>2+</sup> and Cd<sup>2+</sup> cationized serine complexes: infrared multiple photon dissociation spectroscopy and density functional theory investigations

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 Correction for 'Zn<sup>2+</sup> and Cd<sup>2+</sup> cationized serine complexes: infrared multiple photon dissociation spectroscopy and density functional theory investigations' by Rebecca A. Coates *et al.*, *Phys. Chem. Chem. Phys.*, 2016, **18**, 22434–22445.

Although the overall conclusions of the original article remain unaffected (no experimental or theoretical IR spectra are changed, nor is any calculated thermochemistry at 0 K), the thermal corrections to the Gibbs free energy at 298 K were mistakenly overestimated. Corrected 298 K free energies are given below in Tables 1, 3 and 4 from the original manuscript. Because the 298 K values were only slightly modified from the published values, we have not corrected the many references to relative energies in the text, except those noted below. Using the correct values, the ion population analysis for the two lowest energy isomers of the [Zn(Ser-H)ACN]<sup>+</sup> complex is altered. Using the correct 298 K ion population analysis, the following corrections are made to the publication.

**Table 1** Relative free energies at 298 K kJ mol<sup>−1</sup> of [Zn(Ser-H)ACN]<sup>+</sup> conformers<sup>a</sup>

Structure	B3LYP	B3LYP-GD3BJ	B3P86	MP2(full)
[N,CO,O <sup>−</sup> ]tgg	0.0	0.0	0.0	1.7
[N,CO <sup>−</sup> ,OH]ggt	2.4	0.2	4.5	0.0
[N,CO,O <sup>−</sup> ]cgg	25.0	24.2	24.6	27.4
[N,O <sub>s</sub> <sup>−</sup> ]tgt	38.4	42.6	44.1	47.9
[N,CO <sup>−</sup> ]tgt	37.5	41.4	43.5	45.1
[N,CO <sup>−</sup> ]gtt	35.6	39.3	41.7	44.4
[N,OH,O <sup>−</sup> ]tgg	41.2	39.8	44.8	40.3
[CO <sup>−</sup> ,O <sup>−</sup> ]ctc <sup>b</sup>	49.2	51.5	54.0	56.5
[CO,O <sup>−</sup> ]etc	56.6	61.5	61.1	66.6
[N,CO <sup>−</sup> ]tgg	54.4	57.9	60.0	65.1
[N <sup>−</sup> ,CO,OH]tggt	58.0	59.2	60.5	57.2
[CO,O <sup>−</sup> ]tgg	58.8	64.5	66.9	77.2
[CO,O <sup>−</sup> ]tgg	59.3	65.2	67.3	77.0
[CO,O <sup>−</sup> ]ttg	59.5	63.9	67.9	78.1
[N <sup>−</sup> ,CO]tggg	65.0	70.5	70.2	73.7
[CO <sub>2</sub> <sup>−</sup> ]ggg	73.9	85.4	81.7	88.5
[CO <sub>2</sub> <sup>−</sup> ]ggt	77.0	89.9	86.3	90.7
[CO <sup>−</sup> ,O]cgt	72.8	73.9	79.1	80.2
[CO <sub>2</sub> <sup>−</sup> ]gtg	80.6	93.8	88.8	100.9
[OH,O <sup>−</sup> ]tgg	112.3	117.1	124.8	126.4

<sup>a</sup> Calculations performed at the stated level of theory using a 6-311+G(2d,2p) basis set. Geometries and vibrational frequencies calculated at the B3LYP/6-311+G(d,p) level. s = side-chain. <sup>b</sup> Salt bridge between NH<sub>3</sub><sup>+</sup> and COO<sup>−</sup> groups.

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**Table 3** Relative free energies at 298 K kJ mol<sup>-1</sup> of low-lying conformers of [Zn(Ser-H)]<sup>+</sup><sup>a</sup>

Structure	B3LYP	B3LYP-GD3BJ	B3P86	MP2(full)
[N,CO,O <sup>-</sup> ]tgg	0.0	0.0	0.0	0.0
[N,CO <sup>-</sup> ,OH]gggt	15.0	13.4	17.9	10.0
[N,CO,O <sup>-</sup> ]cgg	21.7	21.2	21.2	21.9
[N,O <sub>s</sub> <sup>-</sup> ]tgt	45.7	48.6	53.6	54.4
[N,CO <sup>-</sup> ]gggt	58.1	60.7	66.1	63.0
[N,OH,O <sup>-</sup> ]tgg	45.5	43.7	49.8	41.7
[CO <sup>-</sup> ,O <sup>-</sup> ]ctc <sup>b</sup>	47.6	49.3	54.1	53.4
[CO,O <sup>-</sup> ]ctc	66.8	70.8	70.8	84.6
[N <sup>-</sup> ,CO,OH]tggt	51.1	52.4	54.4	52.5
[CO <sub>2</sub> <sup>-</sup> ]ggg	95.1	106.6	113.2	148.2

<sup>a</sup> Calculations performed at the stated level of theory using a 6-311+G(2d,2p) basis set. Geometries and vibrational frequencies calculated at the B3LYP/6-311+G(d,p) level. s = side-chain. <sup>b</sup> Salt bridge between NH<sub>3</sub><sup>+</sup> and COO<sup>-</sup> groups.

**Table 4** Relative free energies at 298 K kJ mol<sup>-1</sup> of CdCl<sup>+</sup>(Ser) conformers<sup>a</sup>

Structure	B3LYP	B3LYP-GD3BJ	B3P86	MP2(full)
[N,CO,OH]tggt	0.0	0.0	0.0	0.0
[N,CO]tcgt	12.0	17.8	13.7	23.1
[CO <sub>2</sub> <sup>-</sup> ]cgg <sup>b</sup>	13.9	25.6	16.9	27.0
[N,CO]tggt	17.4	22.4	19.0	28.5
[CO <sub>2</sub> <sup>-</sup> ]cggt <sup>b</sup>	15.7	28.0	19.7	30.6
[N,CO]tgtg	19.0	23.7	20.6	31.2
[N,OH <sub>s</sub> ]tggt	24.5	28.8	27.5	31.8
[N,CO,OH]cggt	28.2	27.8	27.8	29.6
[N,OH,OH]tggt	29.4	27.8	31.7	26.4
[N,OH <sub>s</sub> ]tttt	33.7	38.1	37.6	41.7
[CO,OH <sub>s</sub> ]cggt	41.9	48.4	44.3	60.2
[N,CO]tcgg	43.6	50.2	45.3	59.7
[COOH]cggt	45.6	58.6	48.0	66.2
[CO <sub>2</sub> <sup>-</sup> ]cggg <sup>b</sup>	45.3	56.8	49.0	62.5
[N,OH]ttgt	53.6	57.8	57.4	59.4
[CO,OH <sub>s</sub> ]lggt <sup>b</sup>	58.0	63.2	59.3	71.5
[CO,OH <sub>s</sub> ]ttgt	57.6	63.5	64.3	78.3
[N,OH]tttt	58.0	62.7	62.6	62.5
[CO,OH <sub>s</sub> ]ctct	59.7	65.1	62.3	75.9
[CO,OH <sub>s</sub> ]tggt	56.0	63.3	62.3	76.4
[N,OH <sub>s</sub> ]cggt	60.8	64.2	63.2	68.9
[O <sub>s</sub> <sup>-</sup> ]cggt <sup>c</sup>	60.8	72.4	64.3	75.5
[OH <sub>s</sub> ]ttcc	99.0	111.1	103.8	124.4
[OH,OH]tggt	112.7	117.9	122.7	127.5
[OH <sub>s</sub> ]tggt	131.3	143.5	141.3	154.6

<sup>a</sup> Calculations performed at the stated level of theory using a def2-TZVPP basis set. Geometries and vibrational frequencies calculated at the B3LYP/def2-TZVP level. s = side-chain. <sup>b</sup> Salt bridge between NH<sub>3</sub><sup>+</sup> and COO<sup>-</sup> groups. <sup>c</sup> Salt bridge between NH<sub>3</sub><sup>+</sup> and O<sub>s</sub><sup>-</sup> groups.

Page 22438, second paragraph, corrected: “In contrast, as seen in Table 1, the presence of the ACN ligand stabilizes the [N,CO<sup>-</sup>,OH]gggt conformer such that it would populate between 14–48% of ions at 298 K.”

Page 22440, seventh paragraph, corrected: “This result is consistent with the relative free energies calculated at the MP2(full) level of theory, which indicate that [N,CO,O<sup>-</sup>]tgg can account for 33% of an equilibrated ion population at 298 K.” In the published manuscript, we concluded that a superposition of the [N,CO,O<sup>-</sup>]tgg and [N,CO<sup>-</sup>,OH]tgg linear IR spectra best agreed with the experimental spectrum, a conclusion that still holds true. Indeed, as the previous [N,CO,O<sup>-</sup>]tgg ion population was calculated to be 52%, the corrected value of 33% agrees more favorably with the relative intensities observed in the experimental spectrum.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

